

Application of the Inner Product Technique to Some Nonpolynomial Potentials for Multidimensional Quantum Systems

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The energy levels of two- and three-dimensional systems are calculated for some nonpolynomial potentials using the inner product technique over a wide range of values of the perturbation parameters. The numerical results for some special cases agree with those of previous workers where available. © 1996 Academic Press, Inc.

1. INTRODUCTION

There are a variety of techniques which have been employed to calculate and to investigate the one-dimensional potentials

$$V(x; \lambda, g) = x^2 + \frac{\lambda x^2}{(1 + gx^2)} \quad (1)$$

$$V(x; g, \alpha) = \frac{1}{2} x^2 + \frac{gx^4}{(1 + \alpha gx^2)}. \quad (2)$$

The potential given by Eq. (1), has recently been studied by many authors using different techniques. Mitra [1] calculated the ground state and first two excited states using the Ritz variational method in combination with a Givens–Householder matrix eigenvalue algorithm. Galicia and Killingbeck [2] used the finite difference method to compute the energy eigenvalues for the three lowest even parity states. Kaushal [3] has obtained the asymptotic expansions for the eigenenergies and eigenfunctions for the potential by expanding the factor $1/(1 + gx^2)$ as a power series in gx^2 . Bessis and Bessis [4] have studied the same problem by taking advantage of a two-parameter (λ and g) scale transformation. Hautot [5] has used a Hill determinant method to calculate the energy eigenvalues. Lai and Lin [6] and Witwit [7] have applied the Hellmann–Feynman and hypervirial theorem and used Padé approximants to calculate the energy eigenvalues from the perturbation series. Fack and Vanden Berghe [8] used the finite difference method in combination with matrix diagonalization for a numerical computation. Hodgson [9] has applied an analytic continuation technique with Taylor series to pro-

duce eigenvalues for wide ranges of perturbation parameters ($0.1 \leq g, \lambda \leq 10^2$) and state number n , and obtained results with very high accuracy.

A set of exact solutions has been found by Flessas [10] under the conditions $\lambda < 0$ and $\lambda = \lambda(g)$. Whitehead *et al.* [11] have proved the existence of a class of exact eigenvalues, when certain algebraic relations between λ and g hold.

As summarized by Mitra [1], this type of interaction occurs in several areas of physics. In particular, this type of potential occurs when considering models in laser theory [12] and also to a zero-dimensional field theory with a nonlinear Lagrangian [13].

The potential 2 has been studied by Auberson [14], who has shown that the perturbation expansion of the eigenvalues E in terms of g , at fixed α , is Borel summable. For the validity of this result, it is essential that the potential $V^\pm(x; g)$ be positive for all “physical” values of g and α , where the “physical” range of the parameters (g and α) is as follows: for the potential $V^+(x; g)$, $g \geq 0$, $\alpha > 0$, and for $V^-(x; g)$, $g \geq 0$, $\alpha > 2$ (in order that $V^-(x, g) \rightarrow \infty$ as $x^2 \rightarrow \infty$). Auberson and Boissiere [15] calculated the ground state energy level for a large range of values of α and g , using several methods. Flessas [16] investigated the same potential, showing that there exists a class of exact eigenvalues and eigenfunctions when certain algebraic relations between g and α hold, with both g and α positive.

Witwit and Killingbeck [17] have applied the Hellmann–Feynman and hypervirial theorems to calculate the energy levels for some limited values of α and g . Handy *et al.* [18] have applied the eigenvalue moment method to calculate energy levels for various values of g and α .

The abundance of studies of one dimensional systems does not carry over to two- and three-dimensional systems, and there are few reported results in the literature, for example Handy *et al.* [18] have applied the eigenvalue moment method to calculate the energy levels for several eigenstates (n_r, l) and for various combinations of the parameters λ and g . Varshni [19] and Roy *et al.* [20] have used the $1/N$ expansion technique to calculate the energy

eigenvalues for many eigenstates for sets of parameters; $0 \leq n_r \leq 2$, $0 \leq l \leq 4$, (λ , $g = 0.1$ to 1000). Finally Witwit [21] has applied the Hellmann–Feynman and hypervirial theorem to calculate the energy eigenvalues for a wide range of the perturbation parameters g and λ .

The inner product method of eigenvalue calculation investigated by many workers and applied to several polynomial potentials in one, two, and three dimensions. We have since established that the method can be modified and extended to treat nonpolynomial potential in more than one dimension. The paper is intended to point out the flexibility of the inner product perturbation theory, which gives it an advantage over previous applications to handle simple polynomial potentials [18, 23, 24].

In the present paper we shall employ the inner product technique to calculate the energy eigenvalues of a nonpolynomial oscillator represented by the following potentials:

$$V(x, y; g, \lambda) = x^2 + y^2 + \lambda[x^2 + y^2][1 + g(x^2 + y^2)]^{-1} \quad (3)$$

$$V^\mp(x, y; g, \alpha) = \frac{1}{2}[x^2 + y^2] \mp g[x^4 + y^4] [1 + g\alpha(x^2 + y^2)]^{-1} \quad (4)$$

$$V(x, y, z; g, \lambda) = x^2 + y^2 + z^2 + \lambda[x^2 + y^2 + z^2] [1 + g(x^2 + y^2 + z^2)]^{-1} \quad (5)$$

$$V^\mp(x, y, z; g, \alpha) = \frac{1}{2}[x^2 + y^2 + z^2] \mp g[x^4 + y^4 + z^4] [1 + g\alpha(x^2 + y^2 + z^2)]^{-1}. \quad (6)$$

The nonpolynomial potentials given by Eqs. (3)–(6) in two and three dimensions are in general nonseparable in Cartesian coordinates, showing symmetrical behavior and, due to this behavior we do not require a great deal of computation to arrive at our results.

The perturbation calculation for the potentials (3)–(6) is made by expanding the factors $f(x, y; g) = [1 + g(x^2 + y^2)]^{-1}$ and $f(x, y, z; g) = [1 + g(x^2 + y^2 + z^2)]^{-1}$ as a power series in $g(x^2 + y^2)$ and $g(x^2 + y^2 + z^2)$ which is valid for $g(x^2 + y^2) \leq 1$ and $g(x^2 + y^2 + z^2) \leq 1$. As $x_1(x_1 = x, y_2 = y, z_3 = z)$ varies from $(-\infty \leq x_1 \leq +\infty)$, the functions $f(x, y; g)$ and $f(x, y, z; g)$ equal zero at the endpoints, and one at the origin, the functions $f(x, y; g)$ and $f(x, y, z; g)$ being always nonnegative.

The complex singularities for the rational fraction potential in Eqs. (3), (5), $x, y, z = \mp i/\sqrt{g}$, will affect the tightness of the bounds, particularly as the poles get closer to the real axis. It has been shown by Handy [22] that mapping the singularities to infinity improves the tightness of the bounds. For large values of g , the perturbing potential is almost entirely concentrated near the origin. The potentials' shapes are controlled by the parameters λ , g , and α (see Fig. 1).

The energy perturbation series is expected to be divergent, so we start by introducing a renormalization parameter (β), so transforming the potential in Eq. (3) to the

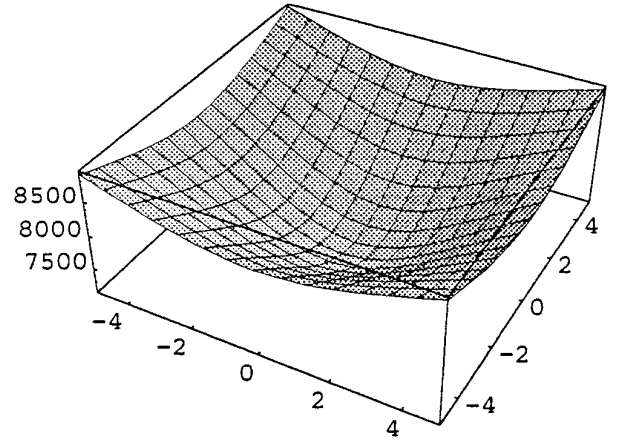


FIG. 1. Nonpolynomial potential $V(x, y, z = 5; \lambda = 10^3, g = 0.1)$.

renormalized form. The potential $V(x, y; \lambda, g)$ in Eq. (3) can be expanded and rewritten in renormalized form:

$$\begin{aligned} V(x, y; \lambda, g, \beta) = & \mu^2[x^2 + y^2] - \lambda\beta[x^2 + y^2] - \lambda g[x^4 + 2x^2y^2 \\ & + y^4] + \lambda g^2[x^6 + 3x^4y^2 + 3x^2y^4 + y^6] \\ & - \lambda g^3[x^8 + 4x^6y^2 + 6x^4y^4 + 4x^2y^6 + y^8] \\ & + \lambda g^4[x^{10} + 5x^8y^2 + 10x^6y^4 + 10x^4y^6 \\ & + 5x^2y^8 + y^{10}] - \lambda g^5[x^{12} + 6x^{10}y^2 + 15x^8y^4 \\ & + 20x^6y^6 + 15x^4y^8 + 6x^2y^{10} + y^{12}] \\ & + \lambda g^6[x^{14} + 7x^{12}y^2 + 21x^{10}y^4 + 35x^8y^6 \\ & + 35x^6y^8 + 21x^4y^{10} + 7x^2y^{12} + y^{14}] \\ & - \lambda g^7[x^{16} + 8x^{14}y^2 + 28x^{12}y^4 + 56x^{10}y^6 \\ & + 70x^8y^8 + 56x^6y^{10} + 28x^4y^{12} + 8x^2y^{14} + y^{16}] \quad (7) \\ & + \lambda g^8[x^{18} + 9x^{16}y^2 + 36x^{14}y^4 + 84x^{12}y^6 \\ & + 126x^{10}y^8 + 126x^8y^{10} + 84x^6y^{12} + 36x^4y^{14} \\ & + 9x^2y^{16} + y^{18}] - \lambda g^9[x^{20} + 10x^{18}y^2 + 45x^{16}y^4 \\ & + 120x^{14}y^6 \\ & + 210x^{12}y^8 + 252x^{10}y^{10} + 210x^8y^{12} \\ & + 110x^6y^{14} + 45x^4y^{16} + 10x^2y^{18} + y^{20}] \\ & - \lambda g^{10}[x^{22} + 11x^{20}y^2 + 55x^{18}y^4 + 165x^{16}y^6 \\ & + 330x^{14}y^8 + 462x^{12}y^{10} + 462x^{10}y^{12} + 330x^8y^{14} \\ & + 165x^6y^{16} + 55x^4y^{18} + 11x^2y^{20} + y^{22}], \end{aligned}$$

where

$$\mu = \sqrt{1 + \lambda + \beta\lambda}, \quad \lambda = 1. \quad (8)$$

Also the nonpolynomial potential $V(x, y, z; g, \lambda)$ in three dimensions can be expanded and rewritten in renormalized form:

$$\begin{aligned} V(x, y, z; \lambda, g, \beta) = & \mu^2[x^2 + y^2 + z^2] - \lambda\beta[x^2 + y^2 + z^2] \\ & - 2\lambda g[x^2y^2 + x^2z^2 + y^2z^2] - \lambda g[x^4 + y^4 + z^4] \\ & + 3g^2\lambda[y^4z^2 + y^4x^2 + y^2z^4 + y^2x^4 + z^4x^2 + z^2x^4] \\ & + g^2\lambda[x^6 + y^6 + z^6] - 4g^3\lambda[y^6z^2 + y^6x^2 + y^2z^6 \\ & + y^2x^6 + z^6x^2 + z^2x^6] - 6g^3\lambda[y^4z^4 + y^4x^4 + x^4z^4] \\ & - 12g^3\lambda[y^4z^2x^2 + y^2z^4x^2 + y^2z^2x^4] - g^3\lambda[x^8 \\ & + y^8 + z^8] + 5g^4\lambda[x^2y^8 + y^2z^8 + z^2y^8 + y^2x^8 \\ & + z^8x^2 + z^2x^8] + 10g^4\lambda[y^6z^4 + y^6x^4 + y^4z^6 \end{aligned}$$

$$\begin{aligned}
& + y^4 x^6 + z^4 x^6 + z^6 x^4 + 20g^4 \lambda [y^6 z^2 x^2 + y^2 z^6 x^2 \\
& + y^2 z^2 x^6] + 30g^4 \lambda [y^4 z^4 x^2 + y^4 z^2 x^4 + y^2 z^4 x^4] \\
& + \lambda g^4 [x^{10} + y^{10} + z^{10}] - 6g^5 \lambda [x^{10} y^2 + x^{10} z^2 \\
& + x^2 y^{10} + x^2 z^{10} + y^{10} z^2 + y^2 z^{10}] - 15g^5 \lambda [x^8 y^4 \\
& + x^8 z^4 + x^4 y^8 + x^4 z^8 + y^8 z^4 + y^4 z^8] \\
& - 30g^5 \lambda [x^8 y^2 z^2 + x^2 y^8 z^2 + x^2 y^2 z^8] \\
& - 60g^5 \lambda [x^6 y^4 z^2 + x^6 y^2 z^4 + x^4 y^6 z^2 + x^4 y^2 z^6 \\
& + x^2 y^6 z^4 + x^2 y^4 z^6] - 20g^5 \lambda [x^6 y^6 + x^6 z^6 + y^6 z^6] \\
& - 90g^5 \lambda [x^4 y^4 z^4] - \lambda g^5 [x^{12} + y^{12} + z^{12}] + 7g^6 \lambda [x^{12} y^2 \\
& + x^{12} z^2 + x^2 y^{12} + x^2 z^{12} + y^{12} z^2 + y^2 z^{12}] \\
& + 21g^6 \lambda [x^{10} y^4 + x^{10} z^4 + x^4 y^{10} + x^4 z^{10} + y^{10} z^4 \\
& + y^4 z^{10}] + 42g^6 \lambda [x^{10} y^2 z^2 + x^2 y^{10} z^2 + x^2 y^2 z^{10}] \\
& + 35g^6 \lambda [x^8 y^6 + x^8 z^6 + x^6 y^8 + x^6 z^8 + y^8 z^6 \\
& + y^6 z^8] + 140g^6 \lambda [x^6 y^6 z^2 + x^6 y^2 z^6 + x^2 y^6 z^6] \\
& + 210g^6 \lambda [x^6 y^4 z^4 + x^4 y^6 z^4 + x^4 y^4 z^6] \\
& + 105g^6 \lambda [x^8 y^4 z^2 + x^8 y^2 z^4 + x^4 y^8 z^2 + x^4 y^2 z^8 \\
& + x^2 y^8 z^4 + x^2 y^4 z^8] + g^6 \lambda [x^{14} + y^{14} + z^{14}] \\
& - 8g^7 \lambda [x^{14} y^2 + x^{14} z^2 + x^2 y^{14} + x^2 z^{14} + y^{14} z^2 \\
& + y^2 z^{14}] - 28g^7 \lambda [x^{12} y^4 + x^{12} z^4 + x^4 y^{12} \\
& + x^4 z^{12} + y^{12} z^4 + y^4 z^{12}] - 56g^7 \lambda [x^{12} y^2 z^2 \\
& + x^2 y^{12} z^2 + x^2 y^2 z^{12}] - 168g^7 \lambda [x^{10} y^4 z^2 + x^{10} y^2 z^4 \\
& + x^4 y^{10} z^2 + x^4 y^2 z^{10} + x^2 y^{10} z^4 + x^2 y^4 z^{10}] \\
& - 56g^7 \lambda [x^{10} y^6 + x^{10} z^6 + x^6 y^{10} \\
& + x^6 z^{10} \\
& + y^{10} z^6 + y^6 z^{10}] - 280g^7 \lambda [x^8 y^6 z^2 + x^8 y^2 z^6 \\
& + x^6 y^8 z^2 + x^6 y^2 z^8 + x^2 y^8 z^6 + x^2 y^6 z^8] \\
& - 420g^7 \lambda [x^8 y^4 z^4 + x^4 y^8 z^4 + x^4 y^4 z^8] \\
& - 70g^7 \lambda [x^8 y^8 + x^8 z^8 + y^8 z^8] \\
& - 560g^7 \lambda [x^6 y^6 z^4 + x^6 y^4 z^6 + x^4 y^6 z^6] \\
& - \lambda g^7 [x^{16} + y^{16} + z^{16}], \\
& \mu = \sqrt{1 + \lambda + \beta \lambda}, \lambda = 1.
\end{aligned} \tag{9}$$

We have expanded the potentials as given by Eqs. (7) and (9) to a limit in which any term beyond that limit makes no difference to our eigenvalues. For our calculations this limit was reached in 10 and 7 terms for two dimensions and three dimensions, respectively.

In this paper, we have carried out extensive numerical calculations of the energy eigenvalues of nonpolynomial potentials in two and three dimensions over a wide range of λ , g , and α values. We have achieved our objective using the inner product technique, which has not been exploited by any previous worker to treat these types of calculations.

Inner product perturbation theory is used to calculate the energy perturbation series. The series does not converge for arbitrary λ and g , but for sufficiently small values of g/λ and g/α it produces accurate results.

2. THE RECURRENCE RELATIONS FOR THE NONPOLYNOMIAL POTENTIALS $V(X, Y; \lambda, g)$ and $V^*(X, Y; g, \alpha)$ IN A TWO-DIMENSIONAL SYSTEM

To find the recurrence relations which allow us to calculate the eigenvalues of the Schrödinger equation for a nonpolynomial potential in a two-dimensional system,

$$H\Psi(x, y) = E\Psi(x, y), \tag{10}$$

where H stands for the Hamiltonian,

$$H = -\partial_{xx}^2 - \partial_{yy}^2 + V(x, y; g, \lambda), \tag{11}$$

we use the reference function,

$$\Phi(x, y) = [x^{L_x} y^{L_y}] \exp[-\frac{1}{2} \mu (x^2 + y^2)] \tag{12}$$

where μ is a variable real positive parameter and L_x and L_y are nonnegative integers. The next step is to work out the quantity

$$EW(M, N) = \langle \Psi | H x^{2M} y^{2N} | \Phi \rangle, \tag{13}$$

obtained by taking the inner product of the Schrödinger equation (10) with the reference function (12). Where $W(M, N)$ is defined by

$$W(M, N) = \langle \Phi | x^{2M} y^{2N} | \psi \rangle \tag{14}$$

and then substituting the perturbation expansions

$$W(M, N) = \sum_K W(M, N, K) \lambda^K \tag{15}$$

$$E = \sum_J E(J) \lambda^J \tag{16}$$

into the $W(M, N)$ recurrence relation given by Eq. (13), which leads to a recurrence relation for the coefficients (see Appendix A).

The coefficients of the potential V_n in Eq. (7) have been expressed in the recurrence relation (A.1) as ($V_1 = -\lambda g$, $V_2 = \lambda g^2$, $V_3 = -\lambda g^3$, ..., $V_9 = -\lambda g^9$, $V_{10} = \lambda g^{10}$). The unperturbed energy can be expressed as

$$E(0) = \mu [4S_x + 4S_y + 2L_x + 2L_y + 2] \tag{17}$$

and the initial condition imposed on $W(M, N, K)$ is given as

$$W(S_x, S_y, 0) = W(S_y, S_x, 0) = \mp 1, \quad S_x = 0; S_y = 0, 1. \tag{18}$$

We exploited the interchange symmetry between the coordinates $x - y$, if the eigenstates have even or odd symmetry, i.e.,

$$W(M, N, K) = \mp W(N, M, K). \tag{19}$$

The state-labelling indices S_x, S_y, L_x, L_y are used in Eqs. (12)–(20) to pick out the particular state being treated as explained in a previous work [23].

The indices are scanned in the order M, N, K as explained in Ref. [23] and the relation (17) is used to work out $W(M, N, K)$ in terms of lower order elements which are already known. $E(J)$ is found from the relation (17) for the special case $M = S_x, N = S_y$, and the sum on the left-hand side becomes $E(J)$, because of the intermediate

TABLE I

Eigenvalues of a Nonpolynomial Potential $V(x, y; \lambda, g)$ for a Two-Dimensional System, for Several Sets of Perturbation Parameters and Several Eigenstates $(n_x, n_y; \pi)$

$n_x, n_y; \pi$	$\lambda=10^2, g=0.05$	$\lambda=10^3, g=0.1$	$\lambda=10^4, g=0.5$	$\lambda=10^6, g=1.5$
0, 0; +	20.0011202288	63.077841686	199.013834778	1997.00437379
0, 1; +	39.9036252215	125.956359638	397.031515447	3991.01212392
0, 2; +	59.6096645912	188.437183244	593.064426467	5979.03338685
0, 2; -=1, 1	59.7075310555	188.635556544	594.053052971	5982.02325293
1, 3; +	98.7283133082	312.803743494	982.164553164	9946.10636015
1, 3; -=2, 2	99.0196111032	313.395998104	985.107742949	9955.05565784
2, 4; +	137.4558483555	436.376882986	1367.310619672	13901.21998088
2, 4; -=3, 3	137.9374952785	437.359188432	1372.177994509	13916.10160899
3, 5; +	175.7924262366	559.156636472	1748.502869838	17844.37431032
3, 5; -=4, 4	176.4613237793	560.525150071	1755.263899175	17865.16112699
4, 6; +	213.7382092661	681.143039306	2125.741551631	21775.56941003
4, 6; -=5, 5	214.5912423590	682.893906047	2134.365550264	21802.23423253
5, 7; +	251.2933658559	802.336127466	2499.026917277	25694.80534183
5, 7; -=6, 6	252.3274026071	804.465479894	2509.483042941	25727.32094638
6, 8; +	288.4580708178	922.735937574	2868.359223377	29602.08216784
6, 8; -=7, 7	289.6699622461	925.239895659	2880.616474293	29640.42128943
7, 9; +	325.2325056844	1042.342506906	3233.738731048	33497.39995046
7, 9; -=8, 8	326.6190854431	1045.217177928	3247.765943391	33541.53528264
8, 10; +	361.6168590497	1161.155873419	3595.165706061	37380.75875238
8, 10; -=9, 9	363.1749431648	1164.397351838	3610.931551369	37430.66294709
9, 11; +	397.6113269299	1279.176075765	3952.640418983	41252.15863659
9, 11; -=10, 10	399.3377134913	1282.780443092	3970.113401495	41307.80430396
10, 12; +	433.2161131469	1396.403153316	4306.163145339	45111.59966635
10, 12; -=11, 11	435.1075820354	1400.366477985	4325.311599255	45172.95937451

Note: The parity label $\pi = +, -$; even, odd for $x \leftrightarrow y$ interchange symmetry.

normalization convention $W(S_x, S_y, 0) = 1$ which we impose on the algorithm.

Fifty coefficients of the perturbation series for the non-polynomial potential (3) for several energy levels were computed; accordingly we find

$$E_{n_x, n_y}(\lambda, g) = \sum_J E(J)\mathcal{M}^J. \tag{20}$$

The algebraic manipulations needed to derive the required recurrence relation for a nonpolynomial potential $V^\mp(x, y; g, \alpha)$ are similar to those which have been used above in connection with the nonpolynomial potential $V(x, y; \lambda, g)$. The potential $V^\mp(x, y; g, \alpha)$ (4) can be expressed in another form, namely

$$\begin{aligned} V^\mp(x, y; g, \alpha) &\equiv \left[\frac{1}{2} \mp \frac{1}{\alpha} \right] [x^2 + y^2] \\ &\pm \frac{1}{\alpha} [x^2 + y^2][1 + g\alpha(x^2 + y^2)]^{-1} \tag{21} \\ &\equiv \left[\frac{1}{2} \mp \frac{1}{\alpha} \right] [x^2 + y^2] \mp \frac{\alpha^{-1}}{g\alpha} \\ &\pm \frac{\alpha^{-1}}{g\alpha} [1 + g\alpha(x^2 + y^2)]^{-1}. \tag{22} \end{aligned}$$

At first sight, on account of Eq. (21) it would seem that $V^\mp(x, y; g, \alpha)$ is similar to $V(x, y; g, \lambda)$, merely by changing λ to α^{-1} and g to $g\alpha$.

3. THE RECURRENCE RELATION FOR THE NONPOLYNOMIAL POTENTIALS $V(X, Y, Z; \lambda, g)$ AND $V^\mp(X, Y, Z; g, \alpha)$ IN A THREE-DIMENSIONAL SYSTEM

The algebraic manipulations needed to derive the required recurrence relation for a nonpolynomial potential in three dimensions (9) are similar to those which have been derived in the two-dimensional system.

To find the recurrence relations which allow us to calculate the eigenvalues of the Schrödinger equation for a nonpolynomial potential (9),

$$H\Psi(x, y, z) = E\Psi(x, y, z), \tag{23}$$

where H stands for the Hamiltonian

$$H = -\partial_{xx}^2 - \partial_{yy}^2 - \partial_{zz}^2 + V(x, y, z; g, \lambda), \tag{24}$$

we use the reference function

$$\Phi(x, y, z) = [x^{L_x}y^{L_y}z^{L_z}] \exp \left[-\frac{1}{2}\mu(x^2 + y^2 + z^2) \right], \tag{25}$$

TABLE II

Eigenvalues of a Nonpolynomial Potential $V^\pm(x, y; g, \alpha)$ for a Two-Dimensional System, for Several Sets of Perturbation Parameters and Several Eigenstates $(n_x, n_y; \pi)$

$n_x, n_y; \pi^\mp$	$g=5 \times 10^{-4}, \alpha=15$		$g=2 \times 10^{-3}, \alpha=2.5$	
	V^+	V^-	V^+	V^-
0, 0; +	1.00097606888	0.99901974798	1.00390752794	0.99602388852
0, 1; \mp	2.00290441203	1.99707783732	2.01162310521	1.98808375983
0, 2; +	3.00669269513	2.99325033848	3.02678571476	2.97226368298
0, 2; $\bar{=}$ 1, 1	3.00576207877	2.99419246378	3.02305193740	2.97619185127
1, 3; +	5.01684198189	4.98294491198	5.06741235493	4.92896182209
1, 3; $\bar{=}$ 2, 2	5.01417755782	4.98566217046	5.05669162208	4.94060236411
2, 4; +	7.03029622246	6.96921153555	7.12127660111	6.87019543487
2, 4; $\bar{=}$ 3, 3	7.02605429143	6.97356678103	7.10414989707	6.88935621812
3, 5; +	9.04691305497	8.95217281951	9.18782062382	8.79606781138
3, 5; $\bar{=}$ 4, 4	9.04123520554	8.95803834596	9.16480653200	8.82255654389
4, 6; +	11.06655865379	10.93194637428	11.26652711803	10.70668453209
4, 6; $\bar{=}$ 5, 5	11.05957337932	10.93920329527	11.23809073421	10.74030883341
5, 7; +	13.08910706271	12.90864501044	13.35691502899	12.60215348293
5, 7; $\bar{=}$ 6, 6	13.08093116899	12.91718267439	13.32347527921	12.64272095905
6, 8; +	15.11443959247	14.88237693313	15.45853585649	14.48258486726
6, 8; $\bar{=}$ 7, 7	15.10517942752	14.89209237349	15.42047155949	14.52990318963
7, 9; +	17.14244427544	16.85324 59311	17.57097044486	16.34809121471
7, 9; $\bar{=}$ 8, 8	17.13219680756	16.86404334977	17.52862537563	16.40196820324
8, 10; +	19.17301537085	18.82135155958	19.69382618257	18.19878738645
8, 10; $\bar{=}$ 9, 9	19.16186913668	18.83314184262	19.64751333366	18.25903109659
9, 11; +	21.20605291520	20.78678931793	21.82673454888	20.03479057683
9, 11; $\bar{=}$ 10, 10	21.19408885592	20.79948958128	21.77673974121	20.10120939064
10, 12; +	23.24146231279	22.74965082031	23.96934895569	21.85622031114
10, 12; $\bar{=}$ 11, 11	23.22875451383	22.76318398512	23.91593391772	21.92862303225

Note: The parity label $\pi = +, -$; even, odd for $x \leftrightarrow y$ interchange symmetry.

where L_x, L_y , and L_z are nonnegative integers. The next step is to work out the quantity

$$EW(M, N, L) = \langle \Psi | Hx^{2M}y^{2N}z^{2L} | \Phi \rangle, \quad (26)$$

obtained by taking the inner product of the Schrödinger equation (24) with the reference function (25), where $W(M, N, L)$ is defined by

$$W(M, N, L) = \langle \Phi | x^{2M}y^{2N}z^{2L} | \psi \rangle, \quad (27)$$

and then substituting the perturbation expansions,

$$W(M, N, L) = \sum_K W(M, N, L, K) \lambda^K \quad (28)$$

$$E = \sum_J E(J) \lambda^J, \quad (29)$$

into $W(M, N, L)$. The recurrence relation given by Eq. (26) leads to a recurrence relation for the coefficients (see Appendix A). The coefficients of the potential V_n in Eq. (9) have been expressed in the recurrence relation (A.2) as ($V_1 = -2\lambda g, V_2 = -\lambda g, V_3 = 3g^2\lambda, \dots, V_{38} = -560g^7\lambda, V_{39} = -7g^7\lambda$). The unperturbed energy can be expressed as

$$E(0) = \mu[4S_x + 4S_y + 4S_z + 2L_x + 2L_y + 2L_z + 3] \quad (30)$$

and the initial condition imposed on the $W(M, N, L, K)$ is given as

$$W(S_x, S_y, S_z, 0) = W(S_z, S_y, S_x, 0) = W(S_x, S_z, S_y, 0) = 1 \\ S_x = S_y = 0; S_z = 0, 1. \quad (31)$$

We exploited the interchange symmetry between the coordinates x, y, z , if the eigenstates have even symmetry, i.e.,

$$W(M, N, L, K) = W(N, M, L, K) = W(M, L, N, M) \\ = W(N, L, M, K) = W(L, N, M, K) \quad (32) \\ = W(L, M, N, K).$$

The state-labelling indices $S_x, S_y, S_z, L_x, L_y, L_z$ are used in Eqs. (25)–(32) to pick out the particular state being treated as explained in a previous work [24].

The indices are scanned in the order M, N, L, K as explained in Ref. [24] and the relation (A.2) is used to

TABLE III

Eigenvalues of a Nonpolynomial Potential $V(x, y, z; \lambda, g)$ for a Three-Dimensional System, for Several Sets of Perturbation Parameters and Several Eigenstates (n_x, n_y, n_z)

n_x	n_y	n_z	$\lambda=10^2, g=0.05$	$\lambda=10^3, g=0.1$	$\lambda=10^4, g=1$	$\lambda=10^6, g=1.5$
0	0	0	29.9646986319	94.542015961	296.293297540	2994.38282665
0	0	1	49.8179020165	157.320873053	491.341145917	4986.89226591
0	1	1	69.5725143962	219.900410451	684.404277261	6976.40508532
1	1	1	89.2285523126	282.280630886	875.482775717	8962.92128745
0	0	2	69.4260020249	219.603208381	681.483757312	6971.92282282
1	1	3	127.8106230386	405.557979419	1243.131193688	12913.56276165
2	2	2	147.6053895268	468.225418141	1436.811337842	14904.49021579
2	2	4	185.3155025392	589.727612409	1787.198119896	18828.29426063
3	3	3	205.0956835816	772.112226685	1980.281381623	20819.08968118
3	3	5	241.9411884895	652.376453806	2313.691324675	24716.11752747
4	4	4	261.6999362737	834.733816454	2505.895442096	26706.71975359
4	4	6	297.6882601123	952.711944759	2822.617972266	30577.03277136
5	5	5	317.4186800832	1015.297587261	3013.656201386	32567.38050348
5	5	7	352.5573302599	1131.526892453	3313.985532462	36411.04020291

work out $W(M, N, L, K)$ in terms of the lower order elements which are already known. $E(J)$ is found from the relation (A.2) for the special case $I = S_x, J = S_y, L = S_z$ and the sum on the left-hand side becomes $E(J)$, because of the intermediate normalization convention $W(S_x, S_y, S_z, 0) = 1$ which we impose on the algorithm.

Forty coefficients of the perturbation series for the non-polynomial potential (9) for several energy levels were computed; accordingly,

$$E_{n_x, n_y, n_z}(\lambda, g) = \sum_J E(J)\lambda^J. \tag{33}$$

The renormalized series method (hypervirial and renormalization parameters β) [24] can be used to compute

the energy eigenvalues for the Schrödinger equation when potential (3) has a circular symmetry in two dimensions, i.e. $(x = r \sin \theta, y = r \cos \theta, r^2 = x^2 + y^2)$ or when the potential (6) has spherical symmetry in three dimensions, i.e. $(x = r \sin \theta \cos \phi, y = r \sin \theta \sin \phi, z = r \cos \theta, r^2 = x^2 + y^2 + z^2)$.

The general form for the Schrödinger equation in N for two or three dimensions can be written as

$$\left[-\frac{d^2}{dr^2} + \frac{1}{4}(N + 2l - 3)(N + 2l - 1)r^{-2} + V_{N=2,3}(r; \lambda g) \right] \Psi(r) = E\Psi(r). \tag{34}$$

TABLE IV

Eigenvalues of a Nonpolynomial Potential $V(x, y, z; \lambda, -g)$ for a Three-Dimensional System, for Several Sets of Perturbation Parameters and Several Eigenstates (n_x, n_y, n_z)

n_x	n_y	n_z	$g=-0.05, \lambda=10^2$	$g=-0.1, \lambda=10^3$	$g=-0.5, \lambda=5000$	$g=-1.5, \lambda=10^5$
0	0	0	30.3599084284	95.29127091295	214.03787275817	954.3306856372
0	0	1	50.68424695387	159.06913234923	357.98618403289	1594.31842930972
0	1	1	71.13192813490	223.04727305943	502.93959517693	2237.31441321541
1	1	1	91.67904720347	287.22569411753	648.89809170287	2883.32099572595
0	0	2	71.28243483450	223.34946313845	504.46703985972	2241.87025777149
1	1	3	133.2825212041	417.09632410941	948.48321338846	4198.7610308047
2	2	2	153.91715612176	480.96264983491	1092.80394997197	4839.40409183883
2	2	4	196.67607413714	612.64519882062	1401.63806518014	6181.76583551447
3	3	3	217.05064366187	676.50216555524	1545.75506330366	6822.58170728583
3	3	5	260.72616170812	810.02307374549	1863.93024401105	8192.63748573201
4	4	4	281.07981710314	873.84426731354	2007.75105436941	8832.85320542641
4	4	6	325.67875893832	1009.20293452207	2335.35843495376	10230.78912443672
5	5	5	346.00496622075	1072.98897978908	2478.79155277915	10870.21796217655
5	5	7	391.3409438415	1210.19376600849	2815.92135791193	12296.1886104439

TABLE V

Eigenvalues of a Nonpolynomial Potential $V^{\pm}(x, y, z; g, \alpha)$ for a Three-Dimensional System, for Several Sets of Perturbation Parameters and Several Eigenstates (n_x, n_y, n_z)

				V^+			
n_x	n_y	n_z	$g=5 \times 10^{-4}, \alpha=15$	$g=10^{-3}, \alpha=10$	$g=2 \times 10^{-3}, \alpha=2.5$	$g=10^{-5}, \alpha=100$	
0	0	0	1.50182265988	1.50360607724	1.50729534072	1.50003736729	
0	0	1	2.50421848253	2.50832022421	2.51687911555	2.50008710193	
0	1	1	3.50753245707	3.51481152383	3.53013039812	3.50015662464	
1	1	1	4.51174282305	4.52302254126	4.54696079930	4.50024587533	
0	0	2	3.50891205065	3.51748609748	3.53566918388	3.50018630784	
1	1	3	6.52663075961	6.55169388995	6.60660074840	6.50057156736	
2	2	2	7.52954565854	7.55743987920	7.61809980227	7.50063139829	
2	2	4	9.55154555764	9.59917807848	9.70637639609	9.50113171600	
3	3	3	10.55470052107	10.60551238515	10.71861537697	10.50119233404	
3	3	5	12.58320443173	12.65885720038	12.83324797041	12.50186518391	
4	4	4	13.58672712055	13.66606693842	13.84665404965	13.50192710003	
4	4	6	15.62119448216	15.72977159110	15.98564648352	15.50277042027	
5	5	5	16.62518921835	16.73807363048	17.00056455267	16.50283413304	
5	5	7	18.66513755734	18.81106576769	19.16255809341	18.50384589300	
6	6	6	19.66968931231	19.82062263898	20.17886559392	19.50391188887	
6	6	8	21.71468648603	21.90197389262	22.36149129414	21.50509008844	
7	7	7	22.71986412426	22.91290576619	23.38022029435	22.50515884204	
7	7	9	24.76952181089	25.00180770046	25.58248219865	24.50650151112	
8	8	8	25.77538074446	26.01420151980	26.60341562777	25.50657348548	
8	8	10	27.82934894471	28.10994640369	28.82405715484	27.50807868342	
9	9	9	28.83593331817	29.12386292447	29.84734567746	28.50815433029	
9	9	11	30.89389568488	31.22582819577	30.08523201835	30.50982014536	
10	10	10	31.90124018282	32.24130746445	33.11099784955	31.50989990545	
10	10	12	33.96291003256	34.34894304012	35.36509964248	33.51172445430	

				V^-			
n_x	n_y	n_z	$g=5 \times 10^{-4}, \alpha=15$	$g=10^{-3}, \alpha=10$	$g=2 \times 10^{-3}, \alpha=2.5$	$g=10^{-5}, \alpha=100$	
0	0	0	1.49816785352	1.49635697696	1.49254856486	1.49996262862	
0	0	1	2.49575196149	2.49156541859	2.48263100759	2.49991288513	
0	1	1	3.49240155783	3.48493480790	3.46876784302	3.49984334595	
1	1	1	4.48813425671	4.47650789584	4.45097152462	4.49975406889	
0	0	2	3.49100225115	3.48218577736	3.46289358015	3.49981365353	
1	1	3	6.47295945771	6.44677344040	6.38633122136	6.49942823496	
2	2	2	7.47000148739	7.44086155229	7.37411036256	7.49936838498	
2	2	4	9.44741057063	9.39699484038	9.27514803450	9.49886774911	
3	3	3	10.44421534364	10.39049088914	10.26231315600	10.49880711957	
3	3	5	12.41475263065	12.33378460460	12.12970036159	12.49813370932	
4	4	4	13.41119346478	13.32639142271	13.11593995912	13.49807197984	
4	4	6	15.37535862196	15.25801228282	14.95035622943	15.49722761193	
5	5	5	16.37132709735	16.24948578024	15.93536293597	16.49716392769	
5	5	7	18.32957892803	18.17048620197	17.73749542828	18.49615093650	
6	6	6	19.32498278289	19.16062829899	18.72096645732	19.49608500003	
6	6	8	21.27774272182	21.07195729921	20.49150955181	21.49490514606	
7	7	7	22.27250396324	22.06060959265	21.47314715726	22.49483648898	
7	7	9	24.22015928844	23.96312288276	23.21280199451	24.49349168730	
8	8	8	25.21421250086	24.95016101354	24.19231394551	25.49341985209	
8	8	10	27.15711927919	26.84463029159	25.90178790310	27.49191199083	
9	9	9	28.15041011347	27.82995896075	26.87888797141	28.49183653060	
9	9	11	30.08889589709	29.71708048045	28.55889407835	30.49016747135	
10	10	10	31.08137972386	30.70062901151	29.53330253576	31.49008794964	
10	10	12	33.01574601514	32.59103171416	31.18455882429	33.48825952791	

TABLE VI

Comparison of Some Eigenvalues of the Nonpolynomial Potential Which Have Been Calculated by the Inner Product Technique with Those Calculated by Other Workers [18, 19, 21]

g	λ	n_x	n_y	n_z	ℓ	n_r	$E_{n_x n_y n_z}$	$E_{n_x n_y n_z}$ [other]
0.1	0.1	0	0	0	0	0	3.120082	3.1200 [19]
		0	0	1	1	0	5.18637	5.186370029314 [18]
		0	1	1	2	0	7.24396	7.243961840414 [18]
		1	1	1	3	0	9.29436	9.294359110863 [18]
		0	0	2	0	1	7.23102	7.2312 [19]
		1	1	3	1	1	13.3557	13.35573 [21]
0.1	1	0	0	0	0	0	4.07988301	4.0798 [19]
		0	0	1	1	0	6.70423889	6.704238892478 [18]
		0	1	1	2	0	9.26191478	9.2619147807 [18]
		1	1	1	3	0	11.7606209	11.760620962631 [18]
		0	0	2	0	1	9.166567	9.1670 [19]
		1	1	3	1	1	16.417924	14.417924 [21]
0.1	10	0	0	0	0	0	9.6190664122	9.6190 [19]
		0	0	1	1	0	15.8137094351	15.8137094352 [18]
		0	1	1	2	0	21.8360925084	21.836092544 [18]
		1	1	1	3	0	27.6883028640	27.68830288 [18]
		0	0	2	0	1	21.5910055108	21.590 [19]
		1	1	3	1	1	38.3822952772	38.38229527720 [21]
0.1	100	0	0	0	0	0	29.7811911107	29.782 [19]
		0	0	1	1	0	49.3897942966	49.38979427 [18]
		0	1	1	2	0	68.8020611552	68.8020615 [18]
		1	1	1	3	0	88.0180659064	88.0180660 [18]
		0	0	2	0	1	68.5130622345	68.512 [19]
		1	1	3	1	1	125.0155588995	125.01555889954 [21]
1	100	0	0	0	0	0	26.7059656	26.706 [19]
		0	0	1	1	0	42.2375602	42.238 [19]
		0	1	1	2	0	55.977803	55.976 [19]
		1	1	1	3	0	67.960806	67.960 [19]
		0	0	2	0	1	53.839093	53.820 [19]
		1	1	3	1	1	82.7689	82.7689 [21]
0.5	500	0	0	0	0	0	65.3089021331	65.30890213313 [21]
		0	0	1	1	0	107.6218639680	107.62186396802 [21]
		0	1	1	2	0	148.9541949498	148.95419494982 [21]
		1	1	1	3	0	189.3062755849	189.30627558489 [21]
		0	0	2	0	1	147.5465293726	147.54652937260 [21]
		1	1	3	1	1	263.0853100021	263.08531000206 [21]
2	500	0	0	0	0	0	60.13925641	60.13925641 [21]
		0	0	1	1	0	95.5803706	95.5803706 [21]
		0	1	1	2	0	127.3216094	127.3216094 [21]
		1	1	1	3	0	155.3869960	155.3869960 [21]
		0	0	2	0	1	122.8043486	122.8043486 [21]
		1	1	3	1	1	191.212736	191.212736 [21]
1	10^3	0	0	0	0	0	91.2566111103	91.256 [19]
		0	0	1	1	0	149.6563194734	149.656 [19]
		0	1	1	2	0	206.1068054466	206.10 [19]
		1	1	1	3	0	260.6091862445	260.62 [19]
		0	0	2	0	1	203.3632851343	203.36 [19]
		1	1	3	1	1	356.2240866493	356.22408664934 [21]
5	10^3	0	0	0	0	0	78.19245	78.19245 [21]
		0	0	1	1	0	119.3154	119.3154 [21]
		0	1	1	2	0	151.7988	151.7988 [21]
		1	1	1	3	0	175.8756	175.8756 [21]
		0	0	2	0	1	143.3959	143.3959 [21]
		1	1	3	1	1	193.259	193.259 [21]

By studying the form of the Schrödinger equation (34), we found that the form of Eq. (34) can be used in two or three dimensions by making the appropriate choice of l . In three dimensions ($N = 3$) l is the usual angular momentum value (0, 1, 2, ...). In two dimension l is set equal to $|m| - \frac{1}{2}$, where m is the magnetic quantum number. The potential $V_{N=2,3}(r; \lambda, g)$ can be expressed as

$$V_{N=2,3}(r, \lambda, g) = \mu r^2 - \lambda \beta r^2 - \lambda [g r^4 - g^2 r^6 + g^3 r^8 - g^4 r^{10} + g^5 r^{12} - g^6 r^{14} + g^7 r^{16}], \quad (35)$$

where

$$\mu = 1 + \lambda + \beta \lambda, \quad \lambda = 1. \quad (36)$$

The energy levels are then most appropriately characterized by the quantum numbers (n_r, l) rather than (n_x, n_y, n_z). The energies of the unperturbed levels are

$$E(0) = (4n_r + 2m + 2)\sqrt{\mu}, \quad N = 2, \quad (37)$$

$$2n_r + m \equiv n_x + n_y, \quad (38)$$

$$E(0) = (4n_r + 2l + 3)\sqrt{\mu}, \quad N = 3, \quad (39)$$

$$2n_r + l \equiv n_x + n_y + n_z, \quad (40)$$

where n_r is called the radial quantum number and l is the angular momentum.

4. RESULTS AND DISCUSSION

The main purpose of this paper was to show the effectiveness of the inner product technique as applied to various multidimensional quantum problems which have not been treated by this technique before.

The energy levels are calculated for several eigenstates over a wide range of perturbation parameters λ, g , and α .

Calculation of the eigenenergies for the potentials $V(x, y; g, \lambda)$ and $V^\pm(x, y; g, \alpha)$ were carried out for sets of (λ, g, α) values. The levels having $n_x = n_y$ values are degenerate with those odd parity levels which satisfy ($n_x, n_y = n_x + 2$).

In Tables I and II, we present 24 energy levels for potentials 3 and 4 for different values of λ, g , and α ($V(\lambda = 10^2 - 10^6; g = 0.5 - 1.5), V^\pm(g = 5 \times 10^{-4}, 2 \times 10^{-3}; \alpha = 2.5, 15)$).

It should also be mentioned that we have not observed any fundamental difference between the V^+ and V^- cases as we vary the perturbation parameters g and α .

For three-dimensional systems we used the inner product technique to calculate the eigenvalues for the potentials $V(x, y, z; \lambda, g)$ and $V^\pm(x, y, z; g, \alpha)$ for several eigenstates with even-parity such as (0, 0, 0), (1, 1, 1), (0, 0, 2), (1, 1,

3), (2, 2, 2), ..., (10, 10, 10), and (10, 10, 12) and mixed parity such as (1, 0, 0) and (1, 1, 0) over a wide range of λ, g , and α . It is clear from our results listed in Tables III–V that the inner product technique works excellently for these values of λ, g , and α .

We want to remark on one aspect of our calculations: It is clear the inner product technique is capable of dealing with any eigenstate has even- or odd-symmetry, with quantum numbers ($n_r = 0, 1; 2m; |m| = 0, 1, 2, 3, \dots$) for a two-dimensional system and ($n_r = 0, 1; 3l; l = 0, 1, 2, 3, \dots$) for the three-dimensional system.

However, from a practical viewpoint handling even-symmetry eigenstates is preferable, because it is simpler and their computation is more quickly performed than unsymmetrical eigenstates, and requires less memory.

There are some other eigenvalue results available by other methods [18, 19, 21]; consequently it is possible to infer the accuracy of the present results by a direct comparison. In Table VI, comparison has been made for the potential $V(x, y, z; \lambda, g)$ for various values of λ and g and several sets of eigenfunctions; such comparison shows that the present technique is highly accurate. We can say that the accuracy of our listed results in Table VI is very good in comparison with the results of Handy *et al.* [18], Varshni [19], and Witwit [21]. To get the energy eigenvalues of our calculations to agree with the results of Ref. [19], it is necessary to multiply his results by 2, since he used $-\frac{1}{2}\nabla^2$ in his Hamiltonian. In Table VI we present six energy levels for the potential $V(x, y, z; \lambda, g)$ for different values of $\lambda = 0.1$ to 1000 and $g = 0.1$ to 5.

In the present work, we push our numerical analysis as far as possible, and in this respect we go further than other workers [18, 19] in our analysis. We study here two- and three-dimensional systems and we extend our calculation to higher excited states.

For large g, α , and small λ , it is found that the inner product technique underestimates the eigenenergies, because it violates the conditions $g(x^2 + y^2) \leq 1$ and $g(x^2 + y^2 + z^2) \leq 1$, which impose on the expansions given by (7), (9). Therefore the inner product technique depends on the ranges which are used for λ and g if it is to give eigenvalue results of good accuracy; therefore we restricted our calculation to a rather small range of g and a large range of λ .

Since many of our results for these potentials are not available in the literature, it has been found useful to have some check on the calculations. Accordingly, some values which are listed in our tables have been checked by us using other methods of calculation, such as renormalized series.

As a next comment we wish to draw attention to the fact that the inner product calculations and renormalized series calculations agree to about all figures.

Aitken extrapolation is used; it seems that such extrapolation improves the convergence of the perturbation series and gives extra digits of accuracy.

For three successive terms of the sequence of E_n values arising from a perturbation series $E_n \lambda^n$, the Aitken extrapolation formula can be expressed as

$$E_n = \frac{[E_n E_{n+2} - E_{n+1}^2]}{[E_{n+2} - 2E_{n+1} + E_n]} \quad (41)$$

This result is easily remembered, but a more stable form of it is

$$E_n = E_n - \frac{[E_{n+1} - E_n]^2}{[E_{n+2} - 2E_{n+1} + E_n]} \quad (42)$$

The second form of the expression (42) is less prone to roundoff errors when E_n , E_{n+1} , and E_{n+2} are very close together in value. The traditional Aitken transformation serves to handle sequences with errors which form a single geometric progression.

APPENDIX A

$$\begin{aligned} \sum_{J=0}^K E(J)W(M, N, K-J) = & V_1 [W(M+2, N, K-1) + 2W(M+1, N+1, K-1) + W(M, N+2, K-1)] \\ & + V_2 [W(M+3, N, K-1) + 3W(M+2, N+1, K-1) + 3W(M+1, N+2, K-1) + W(M, N+3, K-1)] \\ & V_3 [W(M+4, N, K-1) + 4W(M+3, N+1, K-1) + 6W(M+2, N+2, K-1) + 4W(M+1, N+3, L, K-1) \\ & + W(M, N+4, K-1)] + V_4 [W(M+5, N, K-1) + 5W(M+4, N+1, K-1) + 10W(M+3, N+2, K-1) \\ & + 10W(M+2, N+3, K-1) + 5W(M+1, N+4, K-1) + W(M, N+5, K-1) + W(M, N, L+3, K-1)] \\ & + V_5 [W(M+6, N, K-1) + 6W(M+5, N+1, K-1) + 15W(M+4, N+2, K-1) \\ & + 20W(M+3, N+3, L, K-1) + 15W(M+2, N+4, K-1) + 6W(M+1, N+5, K-1) + W(M, N+6, K-1)] \\ & + V_6 [W(M+7, N, K-1) + 7W(M+6, N+1, K-1) + 21W(M+5, N+2, K-1) + 35W(M+4, N+3, K-1) \\ & + 35W(M+3, N+4, K-1) + 21W(M+2, N+5, K-1) + 7W(M+1, N+6, K-1) + W(M, N+7, K-1)] \\ & + V_7 [W(M+8, N, K-1) + 8W(M+7, N+1, K-1) + 28W(M+6, N+2, K-1) + 56W(M+5, N+3, K-1) + 70 \\ & W(M+4, N+4, K-1) + 56W(M+3, N+5, K-1) + 28W(M+2, N+6, K-1) + 8W(M+1, N+7, K-1) + W(M, N+8, K-1)] \\ & + V_8 [W(M+9, N, K-1) + 9W(M+8, N+1, K-1) + 36W(M+7, N+2, K-1) + 84W(M+6, N+3, K-1) \\ & + 126W(M+5, N+4, K-1) + 126W(M+4, N+5, K-1) + 84W(M+3, N+6, K-1) + 36W(M+2, N+7, L+3, K-1) \\ & + 9W(M+1, N+8, K-1) + W(M, N+9, K-1)] \\ & + V_9 [W(M+10, N, K-1) + 10W(M+9, N+1, K-1) + 45W(M+8, N+2, K-1) + 120W(M+7, N+3, K-1) \\ & + 210W(M+6, N+4, L, K-1) + 252W(M+5, N+5, K-1) + 210W(M+4, N+6, K-1) + 110W(M+3, N+7, K-1) \\ & + 45W(M+2, N+8, K-1) + 10W(M+1, N+9, K-1) + W(M, N+10, K-1)] \\ & + V_{10} [W(M+11, N, K-1) + 11W(M+10, N+1, K-1) + 55W(M+9, N+2, K-1) \end{aligned}$$

$$\begin{aligned}
&+165W(M+8, N+3, K-1)+330W(M+7, N+4, K-1)+462W(M+6, N+5, K-1) \\
&+462W(M+5, N+6, K-1)+330W(M+4, N+7, K-1)+165W(M+3, N+8, K-1) \\
&+55W(M+2, N+9, K-1)+11W(M+1, N+10, K-1)+W(M, N+11, K-1) \\
&-\beta \left[W(M+1, N, K-1)+W(M, N+1, K-1) \right] +\mu \left[4M+4N+2L_x+2L_y+2 \right] W(M, N, K) \\
&\quad -2M \left[2M+2L_x-1 \right] W(M-1, N, K) -2N \left[2N+2L_y-1 \right] W(M, N-1, K) . \tag{A.1}
\end{aligned}$$

$$\begin{aligned}
\sum_{J=0}^K E(J)W(M, N, L, K-J) &=V_1 \left[W(M+1, N+1, L, K-1)+W(M+1, N, L+1, K-1)W(M, N+1, L+1, K-1) \right] \\
&+V_2 \left[W(M+2, N, L, K-1)W(M, N+2, L, K-1)+W(M, N, L+2, K-1) \right] \\
V_3 &\left[W(M, N+2, L+1, K-1)+W(M+1, N+2, L, K-1)+W(M, N+1, L+2, K-1)+W(M+2, N+1, L, K-1) \right. \\
&+W(M+1, N, L+2, K-1)+W(M+2, N, L+1, K-1) \left. \right] +V_4 \left[W(M+3, N, L, K-1) +W(M, N+3, L, K-1) \right. \\
&+W(M, N, L+3, K-1) \left. \right] +V_5 \left[W(M, N+3, L+1, K-1)W(M+1, N+3, L, K-1)+W(M, N+1, L+3, K-1) \right. \\
&+W(M+3, N+1, L, K-1)+W(M+1, N, L+3, K-1)W(M+3, N, L+1, K-1) \left. \right] \\
&+V_6 \left[W(M, N+2, L+2, K-1)+W(M+2, N+2, L, K-1)W(M+2, N, L+2, K-1) \right] +V_7 \left[W(M+1, N+2, L+1, K-1) \right. \\
&+W(M+1, N+1, L+2, K-1)+W(M+2, N+1, L+1, K-1) \left. \right] +V_8 \left[W(M+3, N+3, L+3, K+1) \right] \\
&+V_9 \left[W(M+4, N, L, K-1)+W(M, N+4, L, K-1)+W(M, N, L+4, K-1) \right] +V_{10} \left[W(M, N+4, L+1, K-1) \right. \\
&+W(M+1, N+4, L, K-1)+W(M, N+1, L+4, K-1)+W(M+4, N+1, L, K-1)+W(M+1, N, L+4, K-1) \\
&+W(M+4, N, L+1, K-1) \left. \right] +V_{11} \left[W(M, N+3, L+2, K-1) +W(M+2, N+3, L, K-1)+W(M, N+2, L+3, K-1) \right. \\
&+W(M+3, N+2, L, K-1) +W(M+2, N, L+3, K-1)+W(M+3, N, L+2, K-1) \left. \right] +V_{12} \left[W(M+1, N+3, L+1, K-1)+ \right. \\
&W(M+1, N+1, L+3, K-1)+W(M+3, N+1, L+1, K+1) \left. \right] +V_{13} \left[W(M+1, N+2, L+2, K-1) \right. \\
&+W(M+2, N+2, L+1, K-1) +W(M+2, N+1, L+2, K-1) \left. \right] \\
&+V_{14} \left[W(M+5, N, L, K-1)+W(M, N+5, L, K-1)+W(M, N, L+5, K-1) \right] \\
&+V_{15} \left[W(M+6, N, L, K-1)+W(M, N+6, L, K-1)+W(M, N, L+6, K-1) \right] \\
&+V_{16} \left[W(M+5, N+1, L, K-1)+W(M+5, N, L+1, K-1)+W(M+1, N+5, L, K-1) \right. \\
&+W(M+1, N, L+5, K-1)+W(M, N+5, L+1, K-1)+W(M, N+1, L+5, K-1) \left. \right] \\
&+V_{17} \left[W(M+4, N+2, L, K-1)+W(M+4, N, L+2, K-1)+W(M+2, N+4, L, K-1) \right. \\
&+W(M+2, N, L+4, K-1)+W(M, N+4, L+2, K-1)+W(M, N+2, L+4, K-1) \left. \right] \\
&+V_{18} \left[W(M+4, N+1, L+1, K-1)+W(M+1, N+4, L+1, K-1)+W(M+1, N+1, L+4, K-1) \right]
\end{aligned}$$

$$\begin{aligned}
& +V_{19} \left[W(M+3, N+3, L, K-1) + W(M+3, N, L+3, K-1) + W(M, N+3, L+3, K-1) \right] \\
& +V_{20} \left[W(M+3, N+1, L+2, K-1) + W(M+3, N+2, L+3, K-1) + W(M+2, N+3, L+1, K-1) \right. \\
& \left. + W(M+2, N+1, L+3, K-1) + W(M+1, N+3, L+2, K-1) + W(M+1, N+2, L+3, K-1) \right] \\
& +V_{21} \left[W(M+2, N+2, L+2, K-1) \right] + V_{22} \left[W(M+7, N, L, K-1) + W(M, N+7, L, K-1) + W(M, N, L+7, K-1) \right] \\
& +V_{23} \left[W(M+4, N+1, L, K-1) + W(M+4, N, L+1, K-1) + W(M+1, N+4, L, K-1) + W(M+1, N, L+4, K-1) \right. \\
& \left. + W(M, N+4, L+1, K-1) + W(M, N+1, L+4, K-1) \right] + V_{24} \left[W(M+5, N+2, L, K-1) + W(M+5, N, L+2, K-1) \right. \\
& \left. + W(M+2, N+5, L, K-1) + W(M+2, N, L+5, K-1) + W(M, N+5, L+2, K-1) + W(M, N+2, L+5, K-1) \right] \\
& +V_{25} \left[W(M+4, N+2, L+1, K-1) + W(M+4, N+1, L+2, K-1) + W(M+2, N+4, L+1, K-1) \right. \\
& \left. + W(M+2, N+1, L+4, K-1) + W(M+1, N+4, L+2, K-1) + W(M+1, N+2, L+4, K-1) \right] \\
& +V_{26} \left[W(M+4, N+3, L, K-1) + W(M+4, N, L+3, K-1) + W(M+3, N+4, L, K-1) \right. \\
& \left. + W(M+3, N, L+4, K-1) + W(M, N+4, L+3, K-1) + W(M, N+3, L+4, K-1) \right] \\
& +V_{27} \left[W(M+5, N+1, L+1, K-1) + W(M+1, N+5, L+1, K-1) + W(M+1, N+1, L+5, K-1) \right] \\
& +V_{28} \left[W(M+3, N+3, L+1, K-1) + W(M+3, N+1, L+3, K-1) + W(M+1, N+3, L+3, K-1) \right] \\
& +V_{29} \left[W(M+3, N+2, L+2, K-1) + W(M+2, N+3, L+2, K-1) + W(M+2, N+2, L+3, K-1) \right] \\
& +V_{30} \left[W(M+8, N, L, K-1) + W(M, N+8, L, K-1) + W(M, N, L+8, K-1) \right] \\
& +V_{31} \left[W(M+7, N+1, L, K-1) + W(M+7, N, L+1, K-1) + W(M+1, N+7, L, K-1) \right. \\
& \left. + W(M+1, N, L+7, K-1) + W(M, N+7, L+1, K-1) + W(M, N+1, L+7, K-1) \right] \\
& +V_{32} \left[W(M+4, N+2, L, K-1) + W(M+4, N, L+2, K-1) + W(M+2, N+4, L, K-1) \right. \\
& \left. + W(M+2, N, L+4, K-1) + W(M, N+2, L+2, K-1) + W(M, N+2, L+4, K-1) \right] \\
& +V_{33} \left[W(M+5, N+2, L+1, K-1) + W(M+5, N+1, L+2, K-1) + W(M+2, N+5, L+1, K-1) \right. \\
& \left. + W(M+2, N+1, L+5, K-1) + W(M+1, N+5, L+2, K-1) + W(M+1, N+2, L+5, K-1) \right] \\
& +V_{34} \left[W(M+4, N+1, L+1, K-1) + W(M+1, N+4, L+1, K-1) + W(M+1, N+1, L+4, K-1) \right] \\
& +V_{35} \left[W(M+5, N+3, L, K-1) + W(M+5, N, L+3, K-1) + W(M+3, N+5, L, K-1) \right. \\
& \left. + W(M+3, N, L+5, K-1) + W(M, N+5, L+3, K-1) + W(M, N+3, L+5, K-1) \right] \\
& +V_{36} \left[W(M+4, N+4, L, K-1) + W(M+4, N, L+4, K-1) + W(M, N+4, L+4, K-1) \right] \\
& +V_{37} \left[W(M+4, N+3, L+1, K-1) + W(M+4, N+1, L+2, K-1) + W(M+3, N+4, L+1, K-1) \right. \\
& \left. + W(M+3, N+1, L+4, K-1) + W(M+1, N+4, L+3, K-1) + W(M+1, N+3, L+4, K-1) \right] \\
& +V_{38} \left[W(M+4, N+2, L+2, K-1) + W(M+2, N+4, L+2, K-1) + W(M+2, N+2, L+4, K-1) \right] \\
& +V_{39} \left[W(M+3, N+3, L+2, K-1) + W(M+3, N+2, L+3, K-1) + W(M+2, N+3, L+3, K-1) \right] \\
& -\beta \left[W(M+1, N, L, K-1) + W(M, N+1, L, K-1) + W(M, N, L+1, K-1) \right] \\
& +\mu \left[4M+4N+4L+2L_x+2L_y+2L_z+3 \right] W(M, N, L, K) - 2M \left[2M+2L_x-1 \right] W(M-1, N, L, K) \\
& \quad - 2L \left[2L+2L_y-1 \right] W(M, N-1, L, K) - 2L \left[2L+2L_z-1 \right] W(M, N, L-1, K)
\end{aligned} \tag{A.2}$$

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